3-Pyridinamine

462-08-8 | DTXSID9047461

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.15 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.55e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

Image not found
Thiourea
Measured: 1.87
Predicted: 1.71

Image not found
Thioacetamide
Measured: 2.17
Predicted: 4.22

Image not found
Ethylenediamine
Measured: 16.6
Predicted: 14.9

Image not found
N,N'-Dimethylthiourea
Measured: 9.60
Predicted: 5.74

Image not found
dl-Diepoxybutane
Measured: 11.6
Predicted: 9.80

Image not found
2,2'-Bioxirane
Measured: 11.6
Predicted: 9.80